



KAWASAKI FUNCTION IN APPROXIMATION: A PEDAGOGICAL COMMUNICATION IN THE CONTEXT OF CRITICAL PHENOMENA

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ABSTRACT

Close to the critical point, transports coefficients are revised at one loop self-consistent calculation. In this pedagogical communication, we compare the full Kawasaki function $F(\mathbf{x})$, associated with the transport coefficient, with its approximated form $f(\mathbf{x})$ both analytically and graphically. We conclude that the approximated function $f(\mathbf{x})$ in the critical phenomena is a very good candidate for acceptance and which, due to its simplicity, is advantageous over $F(\mathbf{x})$ and hence preferable in carrying out calculations.

INTRODUCTION

In the study of critical dynamics we turn to the question of how long does it take an order parameter to return to the equilibrium once it is disturbed from it. The approach to equilibrium is governed by Langevin equations. If the order parameter is $\psi(x, t)$, the dynamical equation is given by

$$\frac{\partial \psi(x, t)}{\partial t} = -\Gamma \frac{\delta F}{\delta \psi} + N(x, t) \quad (1)$$

where we take ψ to be scalar but in general ψ is a n-component field. F is the equilibrium free energy functional and Γ is known as Onsager co-efficient. N is the noise coming from the averaging over the short range fluctuations and obeying the fluctuation-dissipation theorem:

$$\langle N(x_2, t_2) N(x_1, t_1) \rangle = 2\Gamma k_B T \delta(x_2 - x_1) \delta(t_2 - t_1) \quad (2)$$

For ψ to be conserved i.e. $\int \psi(\vec{x}, t) d^D x = 0$, Eq.(1) would be modified as

$$\frac{\partial \psi(x, t)}{\partial t} = \Gamma \nabla^2 \frac{\delta F}{\delta \psi} + N(x, t) \quad (3)$$

with

$$\langle N(x_2, t_2) N(x_1, t_1) \rangle = -2\Gamma k_B T \nabla^2 \delta(x_2 - x_1) \delta(t_2 - t_1) \quad (4)$$

It is, however, convenient to work in the Fourier space, in which Eqs.(1), (2), (3) and (4) respectively read as

$$\frac{\partial \psi(k, t)}{\partial t} = -\Gamma \frac{\delta F}{\delta \psi(-k)} + N \quad (5)$$

$$\langle N(k_2, t_2) N(k_1, t_1) \rangle = 2\Gamma k_B T \delta(k_2 + k_1) \delta(t_2 - t_1) \quad (6)$$

$$\frac{\partial \psi(k, t)}{\partial t} = -\Gamma k^2 \frac{\delta F}{\delta \psi(-k)} + N \quad (7)$$

$$\langle N(k_2, t_2)N(k_1, t_1) \rangle = 2\Gamma k^2 k_B T \delta(k_2 + k_1) \delta(t_2 - t_1) \quad (8)$$

The free energy functional, in the Gaussian approximation, is given by

$$F[\psi(k)] = \frac{1}{2} \sum_k (\kappa^2 + k^2) \psi(k) \psi(-k) \quad (9)$$

where $\kappa^2 \propto (T - T_c)$, T_c being the critical temperature. After a little algebra, it can be shown that the time-dependent correlation function in the case of non-conserved order parameter decays in the fashion

$$C(k, t_2 - t_1) = C(k, 0) e^{-\Gamma(\kappa^2 + k^2)(t_2 - t_1)} \quad (10)$$

where $C(k, 0) = \frac{k_B T}{(\kappa^2 + k^2)}$, the equal time correlation function. Eq.(10) shows that a relaxation towards the equilibrium occurs over a time scale $\tau = [\Gamma(\kappa^2 + k^2)]^{-1}$. Hence the characteristic frequency $\omega (= \tau^{-1})$ is given by

$$\omega = \Gamma(\kappa^2 + k^2) = k^z g(x) \quad (11)$$

where $z = 2$ and $g(x) = \Gamma\left(1 + \frac{1}{x^2}\right)$ with $x = \frac{k}{\kappa}$. Eq.(11) shows that for a fixed k when $\kappa \rightarrow 0$ (i.e. $T \rightarrow T_c$), $\omega \sim k^z$ which implies that the relaxation rate is slower for longer wavelengths. This is popularly known as critical slowing down. The exponent z is known as dynamic critical exponent [1,2]. Clearly, for conserved order parameter, $z = 4$. Unfortunately, none of these exponents comes out of experiments. This is because of the fact that the Onsager co-efficient Γ is treated non-critically. If we incorporate non-linear terms in the equation of motion, then Γ comes out to be k and κ dependent. The first non-linearity that comes to our mind is the ψ^4 term in the free energy functional, which in the k -space is given by

$$F[\psi(k)] = \frac{1}{2} \sum_k (\kappa^2 + k^2) \psi(k) \psi(-k) + \frac{u}{4!} \sum_{k_1, k_2, k_3} \psi(-k_1) \psi(-k_2) \psi(-k_3) \psi(-k_1 - k_2 - k_3) \quad (12)$$

where u is the coupling constant. In this case a perturbation expansion in $\epsilon (= 4 - D)$ yields the dynamic exponent $z = 2 + \left(6 \ln \frac{4}{3} - 1\right) \eta + O(\epsilon^3)$ for the non-conserved case and $z = 4 - \eta$ correct to all order in ϵ , for conserved case. Here η is the anomalous dimension. Thus the change produced in the dynamic exponent z is $O(\eta)$ which is $O(10^{-2})$. Hence the effect of this type of dissipative non-linearity is very small.

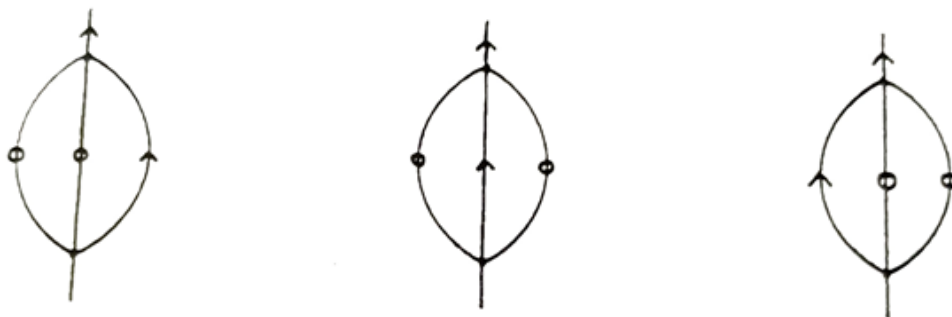


Figure 1: Two loop diagrams for ψ^4 interaction

The important nonlinearities are the reversible term in the equation of motion. It should be kept in mind that the reversible terms are always constructed in such a manner that the equilibrium free energy is left invariant in time (i.e. energy is conserved and that is why these nonlinearities are termed as reversible) and that allows for consistent definition of time dependent equilibrium correlation. If we are dealing with the liquid-gas critical point or the consolute point of a binary liquid, the order parameter for which is the density difference (ρ) from a critical value or the concentration difference (c) from a critical value respectively, then the dynamics of the order parameter is coupled to that of the velocity field through the Eulerian derivative $\frac{d}{dt} = \frac{\partial}{\partial t} + (\vec{v} \cdot \vec{\nabla})$. Accordingly, we consider the equation of motion (binary fluid) is of the form

$$\frac{\partial c}{\partial t} = -(\vec{v} \cdot \vec{\nabla})c \quad (13)$$

The Fourier component $c(k, t)$ satisfies

$$\dot{c}(k) = -i \sum_p \vec{k} \cdot \vec{v}(\vec{p}) c(\vec{k} - \vec{p}) \quad (14)$$

The time dependent correlation function of the order parameter now decays as

$$G_c(k, t_2 - t_1) = \langle c(k, t_2) c(-k, t_1) \rangle = \frac{k_B T}{(\kappa^2 + k^2)} \exp[-Dk^2(t_2 - t_1)] \quad (15)$$

with the decay rate $\tau = Dk^2$, where D is the effective diffusion constant arising from the imposed nonlinearities and is related to the susceptibility χ and concentration transport coefficient λ through the relation $D = \frac{\lambda}{\chi}$. The incompressibility condition $\vec{\nabla} \cdot \vec{v} = 0$ implies that the velocity field is transverse. The time dependent correlation function for the velocity field decays as

$$G_v(k, t_2 - t_1) = \langle v_i(k, t_2) v_j(-k, t_1) \rangle = \frac{k_B T}{m} \delta_{ij} \exp[-\eta k^2(t_2 - t_1)] \quad (16)$$

where η is the shear viscosity. Thus, for the momentum current, the transport coefficient is the shear viscosity η and the corresponding susceptibility is simply the density ρ of the system. The momentum diffusion coefficient is the kinematic viscosity ν and we have $\nu = \frac{\eta}{\rho}$. We now need to discuss what happens to the transport coefficient near the critical point.

Close to the critical point, regions where fluctuations are correlated become very large and the correlation length ξ which characterizes the system becomes infinite at $T = T_c$. If we are in the long wave limit (i.e. $k \cong 0$) and approach the critical point (i.e. start from finite κ and approach $\kappa = 0$), then the excess transport coefficient $\Delta\lambda$ and the excess shear viscosity $\Delta\eta$ coming from the critical fluctuations behave as

$$\Delta\lambda \sim \xi^{x_\psi} \quad (17)$$

$$\Delta\eta \sim \xi^{x_\eta} \quad (18)$$

We note that the divergence of shear viscosity is very weak ($x_\eta = \frac{\epsilon}{19}$ for $\epsilon \ll 1$) [3] and often it is a good approximation to set $x_\eta \cong 0$ to find the concentration transport coefficient $\Delta\lambda$. Moreover, for low k (the long wavelength, in which we are interested), $\Sigma_v \gg \Sigma_\psi$ [(where Σ_v and Σ_ψ are respectively the self-energy for velocity field and order parameter field (Figs.-2 and 3)] for all $D > 2$ and also when the dependence on the external frequency ω is considered, these frequencies are of the order of

the relaxation rate of the order parameter and we will always have $\omega \ll \Sigma_v$. If this is done, then one loop self consistent calculation in the physical dimension $D = 3$ yields [2,4]

$$\Delta\lambda(k, \kappa) = \frac{1}{\eta} \int \frac{d^3p}{(2\pi)^3} \frac{\sin^2\theta}{(p^2 + \kappa^2)} \frac{1}{(\vec{k} - \vec{p})^2} \quad (19)$$

where θ is the angle between \vec{k} and \vec{p} .

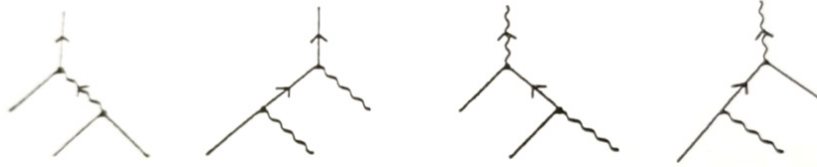


Figure 2: Second order tree diagrams for the order parameter and transverse momentum expansion. The straight lines represent the order parameter and the wavy lines for transverse momentum.

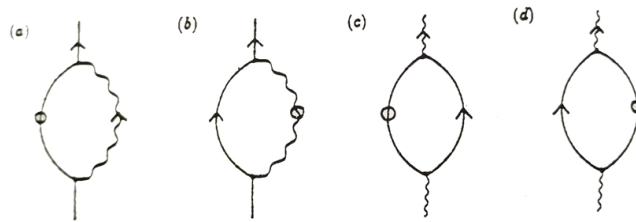


Figure 3: One loop order corrections for order parameter and transverse momentum correlation functions. The solid lines stand for density fluctuation and the wavy lines for velocity fluctuations. Propagators appear with an arrow and correlators with an open circle.

In the limit $\kappa = 0$

$$\Delta\lambda(k) = \frac{1}{\eta k} \int \frac{d^3p}{(2\pi)^3} \frac{\sin^2\theta}{p^2} \frac{1}{(\vec{k} - \vec{p})^2} = \frac{1}{\eta k} \frac{4\pi}{(2\pi)^3} \frac{\pi^2}{8} \quad (20)$$

while in the limit $k = 0$

$$\Delta\lambda(\kappa) = \frac{1}{\eta \kappa} \int \frac{d^3p}{(2\pi)^3} \frac{\sin^2\theta}{(1+p^2)} \frac{1}{p^2} = \frac{1}{\eta \kappa} \frac{4\pi}{(2\pi)^3} \frac{\pi}{3} = \frac{1}{6\pi\eta\kappa} \quad (21)$$

For arbitrary k and κ , we approximately write $\Delta\lambda(k, \kappa)$ by the method of extrapolation as

$$\Delta\lambda(k, \kappa) \cong \frac{1}{6\pi\eta\kappa} \left[1 + \left(\frac{3\pi}{8} \right)^2 \left(\frac{k}{\kappa} \right)^2 \right]^{-1/2} \cong \frac{1}{6\pi\eta\kappa} \left[1 + \left(\frac{k}{\kappa} \right)^2 \right]^{-1/2} = \frac{1}{6\pi\eta\kappa} f(x) \quad (22)$$

where

$$f(x) = \frac{1}{\sqrt{1+x^2}} \quad \text{with } x = \frac{k}{\kappa} \quad (23)$$

However, for arbitrary k and κ , the integral in Eq.(19) can be done exactly and we have

$$\Delta\lambda(k, \kappa) = \frac{1}{6\pi\eta\kappa} F(x) \quad (24)$$

where

$$F(x) = \frac{3}{4x^2} \left[1 + x^2 + \left(x^3 - \frac{1}{x} \right) \tan^{-1}x \right] \quad \text{with } x = \frac{k}{\kappa} \quad (25)$$

The scaling function $F(x)$ is generally known as Kawasaki function. It is to be noted that for the purpose of calculation we use the approximated function $f(x)$ instead of the full Kawasaki function $F(x)$ for the sake of simplicity. This immediately prompts us to make a comparative study of these two functions.

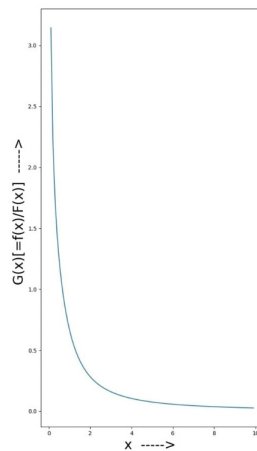


Figure 4: Plot of $G(x) \left[= \frac{f(x)}{F(x)} \right]$ as a function of x .

From the above plot, we see that the discrepancy between these two functions drops as the value of x increases. Since the higher value of x corresponds to $\kappa \rightarrow 0$ or equivalently $T \rightarrow T_c$, the approximated function $f(x)$ in the critical phenomena is a good candidate for acceptance, a point we want highlight in this pedagogical communication.

In closing, it should be noted that we have studied the dynamic critical behaviour of the concentration fluctuations and velocity fluctuations in binary fluids so far. The ordinary fluid near the liquid-vapour critical point is in the same universality class but the order parameter for the liquid-vapour critical point is not a clear density fluctuation but a mixture of density and energy fluctuations – in fact it is very close to the entropy fluctuations. Consequently, ψ stands for the entropy fluctuations, λ is the thermal conductivity and χ denotes the specific heat at constant pressure. The coupling to the velocity fluctuations and the nonlinearity in the velocity equation remain unaltered and Eqs. (17) and (18) imply that the thermal conductivity and shear viscosity diverge near the liquid-vapour critical point.

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